ISOPHYTOL

Other names: 1-Hexadecen-3-ol, 3,7,11,15-tetramethyl-
Hexadec-1-en-3-ol, 3,7,11,15-tetramethyl-
1-Hexadecene-3-ol, 3,7,11,15-tetramethyl
NSC 93744
3,7,11,15-Tetramethylhexadec-1-en-3-ol
2,6,10,14-Tetramethylhexadec-15-en-14-ol
3,7,11,15-Tetramethyl-1-hexadecen-3-ol

Inchi: InChI=1S/C20H40O/c1-7-20(6,21)16-10-15-19(5)14-9-13-18(4)12-8-11-17(2)3/h7,17-19,2

InchiKey: KEVYVLWNCKMXJX-UHFFFAOYSA-N

Formula: C20H40O

SMILES: C=CC(C)(O)CCCC(C)CCCC(C)CCCC(C)C

Mol. weight [g/mol]: 296.54

Physical Properties

Property code	Value	Unit	Source
af	0.8863		Cheméo Relay (1.0)
hfus	32.38	kJ/mol	Joback Method
hvap	97.74	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.40		Cheméo Relay (1.0)
logp	6.362		Crippen Method
mcvol	294.230	ml/mol	McGowan Method
pc	1140.57	kPa	Joback Method
rinpol	1949.00		NIST Webbook
rinpol	1951.00		NIST Webbook
rinpol	1947.00		NIST Webbook
rinpol	1948.00		NIST Webbook
rinpol	1949.00		NIST Webbook
rinpol	1950.00		NIST Webbook
rinpol	1943.00		NIST Webbook
rinpol	1950.00		NIST Webbook
rinpol	1943.00		NIST Webbook
rinpol	1950.00		NIST Webbook
rinpol	1942.00		NIST Webbook
rinpol	1945.00		NIST Webbook
rinpol	1950.00		NIST Webbook
rinpol	1939.00		NIST Webbook
rinpol	1944.00		NIST Webbook

rinpol	1949.00	NIST Webbook
rinpol	1950.00	NIST Webbook
rinpol	1922.00	NIST Webbook
rinpol	1932.00	NIST Webbook
rinpol	1950.00	NIST Webbook
rinpol	1943.00	NIST Webbook
rinpol	1938.00	NIST Webbook
rinpol	1950.00	NIST Webbook
rinpol	1942.00	NIST Webbook
rinpol	1956.00	NIST Webbook
rinpol	1942.00	NIST Webbook
rinpol	1920.00	NIST Webbook
rinpol	1956.00	NIST Webbook
rinpol	1944.00	NIST Webbook
rinpol	1949.00	NIST Webbook
rinpol	1947.00	NIST Webbook
rinpol	1949.00	NIST Webbook
rinpol	1949.00	NIST Webbook
rinpol	1948.60	NIST Webbook
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rinpol	1938.00	NIST Webbook
rinpol	1954.00	NIST Webbook
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rinpol	1943.00	NIST Webbook
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rinpol	1948.00		NIST Webbook
rinpol	1950.00		NIST Webbook
rinpol	1950.00		NIST Webbook
rinpol	1950.00		NIST Webbook
ripol	2282.00		NIST Webbook
ripol	2296.00		NIST Webbook
ripol	2316.00		NIST Webbook
ripol	2278.00		NIST Webbook
ripol	2327.00		NIST Webbook
ripol	2286.00		NIST Webbook
ripol	2282.00		NIST Webbook
ripol	2296.00		NIST Webbook
ripol	2299.00		NIST Webbook
ripol	2296.00		NIST Webbook
ripol	2296.00		NIST Webbook
tb	600.45	K	Cheméo Relay (1.0)
tc	763.71	K	Cheméo Relay (1.0)
tf	279.13	K	Cheméo Relay (1.0)
vc	1.080	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	903.98	J/mol×K	741.31	Joback Method
cpg	923.04	J/mol×K	770.46	Joback Method
cpg	941.17	J/mol×K	799.61	Joback Method
cpg	958.41	J/mol×K	828.75	Joback Method
cpg	974.81	J/mol×K	857.90	Joback Method
cpg	990.43	J/mol×K	887.05	Joback Method
cpg	1005.31	J/mol×K	916.20	Joback Method
dvisc	0.0150671	Pa×s	331.64	Joback Method
dvisc	0.0017320	Pa×s	399.92	Joback Method
dvisc	0.0003742	Pa×s	468.20	Joback Method
dvisc	0.0001194	Pa×s	536.47	Joback Method
dvisc	0.0000493	Pa×s	604.75	Joback Method
dvisc	0.0000244	Pa×s	673.03	Joback Method
dvisc	0.0000137	Pa×s	741.31	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C505328&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

hfus: Enthalpy of fusion at standard conditions

hvap: Enthalpy of vaporization at standard conditions

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

pc: Critical Pressure

rinpol: Non-polar retention indices

ripol: Polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume